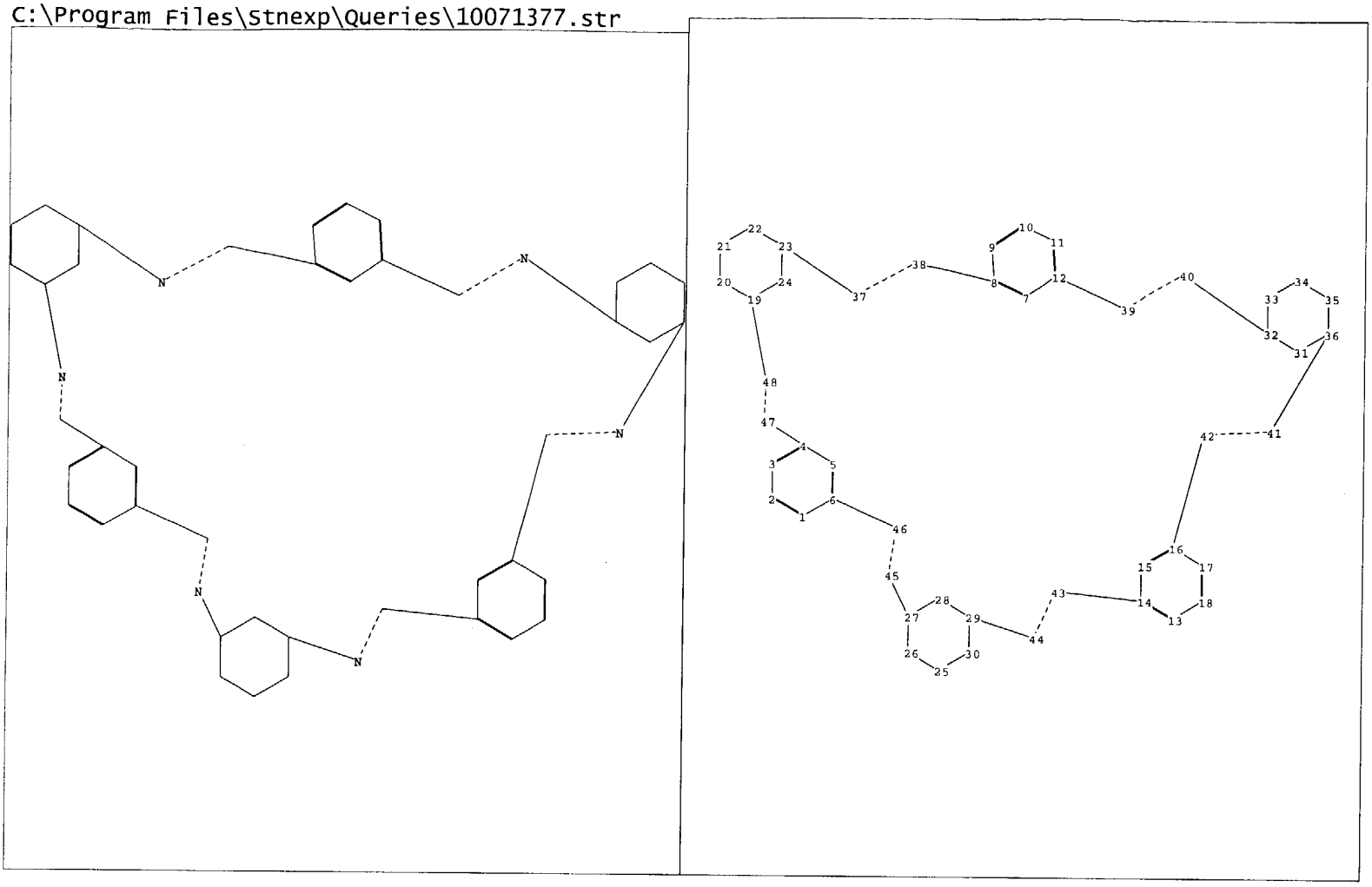
C:\Program Files\Stnexp\Queries\10071377.str



ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48
ring bonds :
1-2 1-6 2-3 3-4 4-5 4-47 5-6 6-46 7-8 7-12 8-9 8-38 9-10 10-11 11-12 12-39
13-14 13-18 14-15 14-43 15-16 16-17 16-42 17-18 19-20 19-24 19-48 20-21 21-22
22-23 23-24 23-37 25-26 25-30 26-27 27-28 27-45 28-29 29-30 29-44 31-32 31-36
32-33 32-40 33-34 34-35 35-36 36-41 37-38 39-40 41-42 43-44 45-46 47-48
exact/norm bonds :
4-47 6-46 8-38 12-39 14-43 16-42 19-20 19-24 19-48 20-21 21-22 22-23 23-24
23-37 25-26 25-30 26-27 27-28 27-45 28-29 29-30 29-44 31-32 31-36 32-33 32-40
33-34 34-35 35-36 36-41 37-38 39-40 41-42 43-44 45-46 47-48
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15
15-16 16-17 17-18

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom 44:Atom 45:Atom 46:CLASS 47:Atom 48:Atom

10/071,377

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=> d his

     (FILE 'HOME' ENTERED AT 11:58:35 ON 02 JUL 2004)

     FILE 'REGISTRY' ENTERED AT 11:58:40 ON 02 JUL 2004
L1                STRUCTURE UPLOADED
L2                QUE L1
L3              2 S L2
L4             19 S L2 SSS FUL

     FILE 'CAPLUS' ENTERED AT 11:59:19 ON 02 JUL 2004
L5              4 S L4

=> d ibib abs hitstr 1-4
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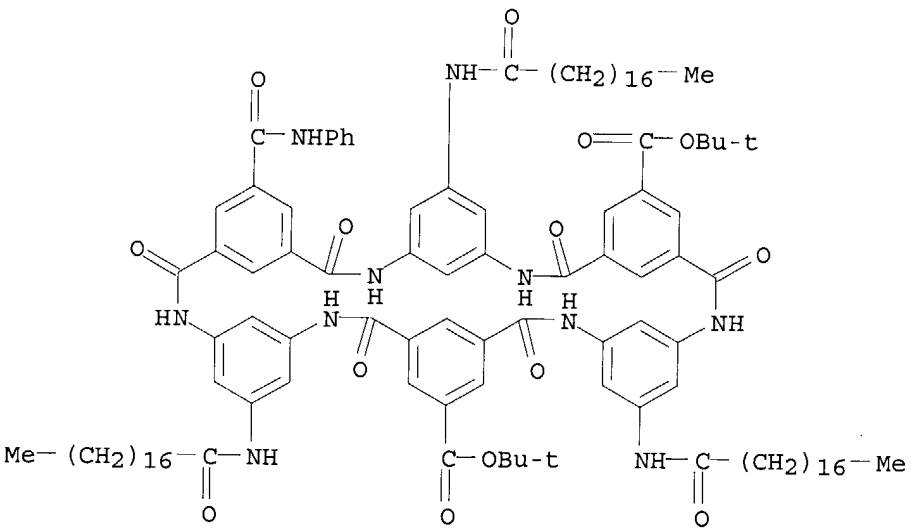
L5 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:51732 CAPLUS
DOCUMENT NUMBER: 140:287366
TITLE: Synthesis of an amide cyclophane building block of shape-persistent triangular molecular wedges
AUTHOR(S): Amma, Achim; Mallouk, Thomas E.
CORPORATE SOURCE: 152 Davey Laboratory, Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Tetrahedron Letters (2004), 45(6), 1151-1153
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of an amide cyclophane, which can be considered as the first generation of a family of triangular shape-persistent mol. wedges, is described.

IT **676127-21-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of an amide cyclophane building block of shape-persistent triangular mol. wedges)

RN 676127-21-2 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-6,20-dicarboxylic acid, 3,9,17,23,31,37-hexaoxo-13,27,41-tris[(1-oxooctadecyl)amino]-34-[(phenylamino)carbonyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

applicant

L5 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:836641 CAPLUS
DOCUMENT NUMBER: 139:337996
TITLE: Preparation of macrocyclic module compositions
INVENTOR(S): Kriesel, Josh; Karpishin, Timothy B.; Bivin, Donald B.; Merrill, Grant; Stuart, Edelstein Martin; Smith, Thomas H.; Whiteford, Jeffery A.; Jonas, Robert Thomas
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 62 pp., Cont.-in-part of U.S. Ser. No. 71,377.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003199688	A1	20031023	US 2002-226400	20020823
US 2004034223	A1	20040219	US 2002-71377	20020207
WO 2003067286	A2	20030814	WO 2003-US3829	20030207
WO 2003067286	A3	20040415		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

WO 2003066646	A2	20030814	WO 2003-US3830	20030207
WO 2003066646	A3	20040212		

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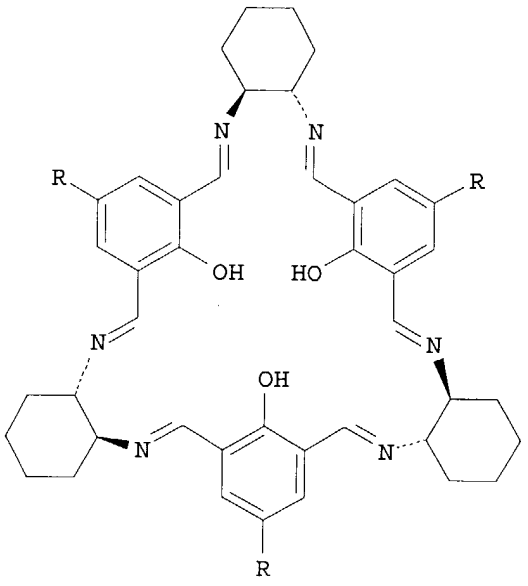
PRIORITY APPLN. INFO.:

US 2002-71377	A2	20020207
US 2002-383236P	P	20020522
US 2002-226400	A	20020823

OTHER SOURCE(S): MARPAT 139:337996
GI



I

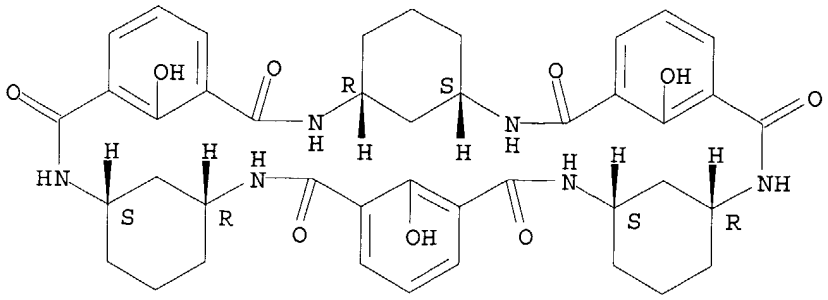
AB Macrocyclic module compns. are made from cyclic synthons. The macrocyclic module structures are prepared by stepwise or concerted schemes which couple synthons in a closed ring. The macrocyclic module structures may have a pore of nanometer dimensions which transports a selected species through the composition Thus, To 0.300 g (1R,2R)-(-)-trans-1,2-diaminocyclohexane (2.63 mmol) in 6 mL CH2Cl2 at 0° was added 0.826 g 2,6-diformyl-4-(1-dodec-1-ynyl)phenol (2.63 mmol) in 6 mL of CH2Cl2. The orange solution was stirred at 0° for 1 h and then allowed to warm to room temperature after which stirring was continued for 16 h, and added to 150 mL methanol. After decanting the methanol solution, a sticky yellow solid. was obtained and purified by chromatog. to give a macrocyclic compound (I; R = 1-dodecyn-1-yl) as a yellow powder. The compound I was inserted into a lipid bilayer formed by phosphatidylcholine and phosphatidylethanolamine. The pore size of the compound I was 3.3 Å. Permeation of various ionic species through the bilayer was tested when a pos. elec. potential was applied to the solution on the side of the lipid bilayer containing the test species. Ionic species such as Na+, K+, Ca2+, NH3+, Cs+, and MeNH3+ were transported through the pore whereas Li+, Mg2+, EtNH3+, NMe4+, NEt4+, aminoguanidine, choline, glucosamine, and NPr4+ were blocked.

IT **615574-19-1 615574-20-4**
RL: PRP (Properties)
(energy-minimized conformations)

RN 615574-19-1 CAPLUS

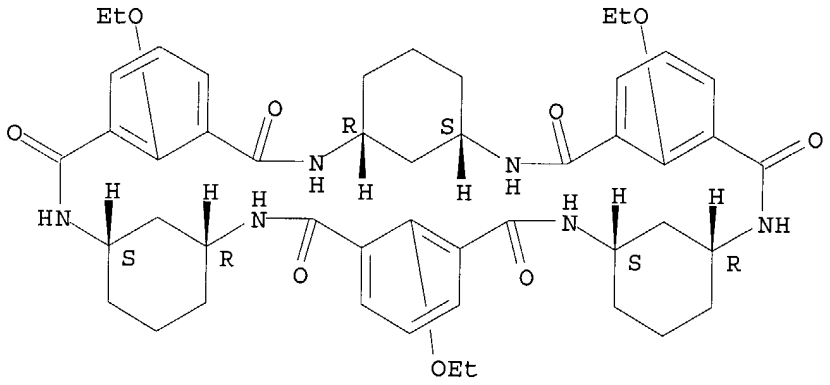
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-4,6,8(48),18,20,22(46),32,34,36(44)-nonaene-3,9,17,23,31,37-hexone, 44,46,48-trihydroxy-, (1R,11S,15R,25S,29R,39S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



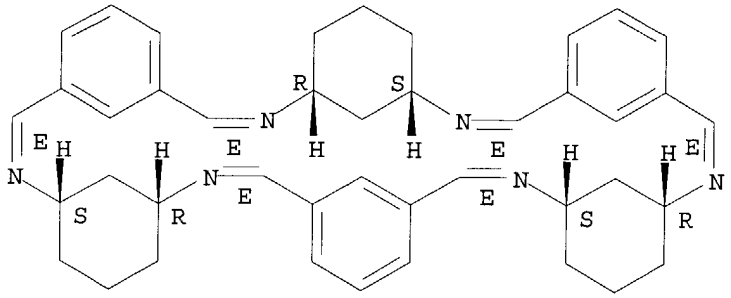
RN 615574-20-4 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-4,6,8(48),18,20,22(46),32,34,36(44)-nonaene-3,9,17,23,31,37-hexone, 44,46,48-triethoxy-, (1R,11S,15R,25S,29R,39S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



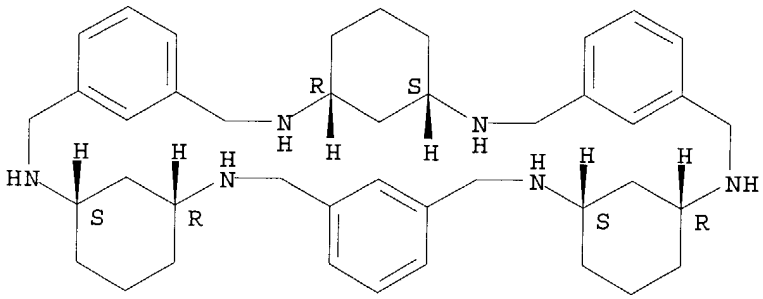
IT **615574-06-6 615574-07-7 615574-08-8 615574-16-8 615574-17-9 616233-21-7 616233-23-9**
RL: PRP (Properties)
(quantum and mol. mech. computations of pore areas)
RN 615574-06-6 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-2,4,6,8(48),9,16,18,20,22(46),23,30,32,34,36(44),37-pentadecaene, (1R,2E,9E,11S,15R,16E,23E,25S,29R,30E,37E,39S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as described by E or Z.



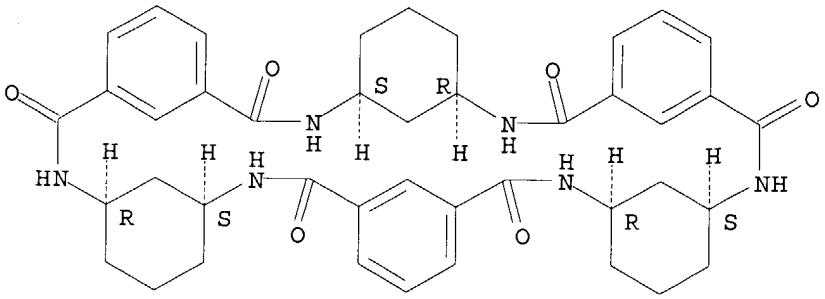
RN 615574-07-7 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-4,6,8(48),18,20,22(46),32,34,36(44)-nonaene, (1R,11S,15R,25S,29R,39S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 615574-08-8 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-4,6,8(48),18,20,22(46),32,34,36(44)-nonaene-3,9,17,23,31,37-hexone, (1R,11S,15R,25S,29R,39S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



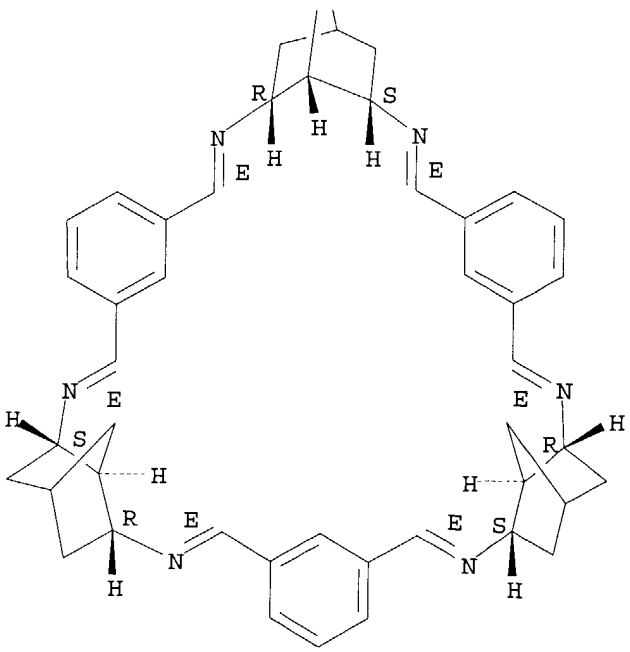
RN 615574-16-8 CAPLUS
CN 2,39:13,15:26,28-Trimethano-6,10:19,23:32,36-trimetheno-10H-tricyclopenta[b,n,z][1,5,13,17,25,29]hexaazacyclohexatriacontine, 1,2,3,3a,13,13a,14,15,16,16a,26,26a,27,28,29,29a,39,39a-octadecahydro-, (3aR,4E,11E,13S,16aR,17E,24E,26S,29aR,30E,37E,39S)-rel- (9CI) (CA INDEX

NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A

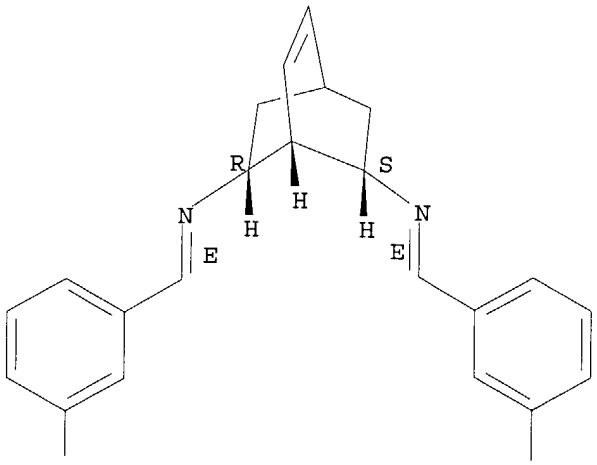
PAGE 2-A



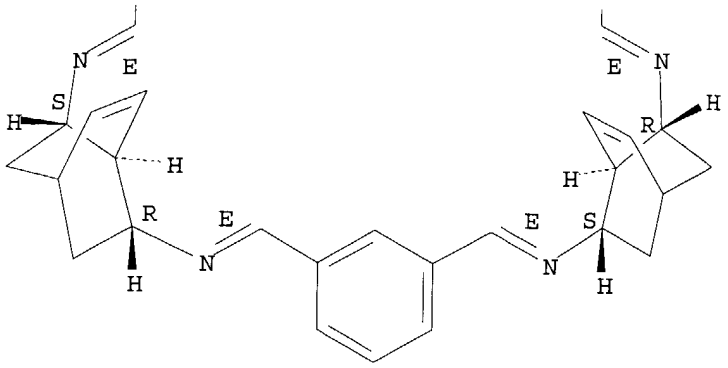
RN 615574-17-9 CAPLUS
CN 3H,14H,28H-3,42:14,17:28,31-Trimethano-7,11:21,25:35,39-trimethenotribenzo[b,n,z][1,5,13,17,25,29]hexaazacyclohexatriacontine, 4,4a,14a,17,18,18a,28a,31,32,32a,42,42a-dodecahydro-, (4aR,5E,12E,14S,18aR,19E,26E,28S,32aR,33E,40E,42S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 2-A



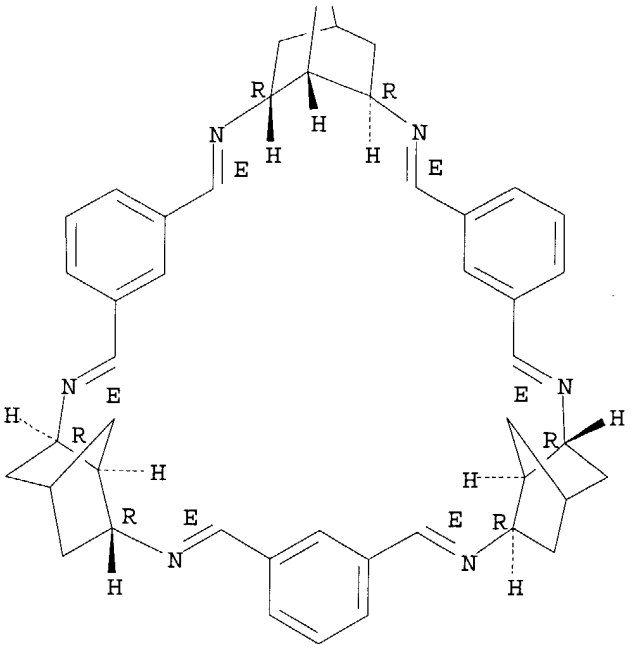
RN 616233-21-7 CAPLUS
CN 2,39:13,15:26,28-Trimethano-6,10:19,23:32,36-trimetheno-10H-tricyclopenta[b,n,z][1,5,13,17,25,29]hexaazacyclohexatriacontine,

1,2,3,3a,13,13a,14,15,16,16a,26,26a,27,28,29,29a,39,39a-octadecahydro-, (3aR,4E,11E,13R,16aR,17E,24E,26R,29aR,30E,37E,39R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A

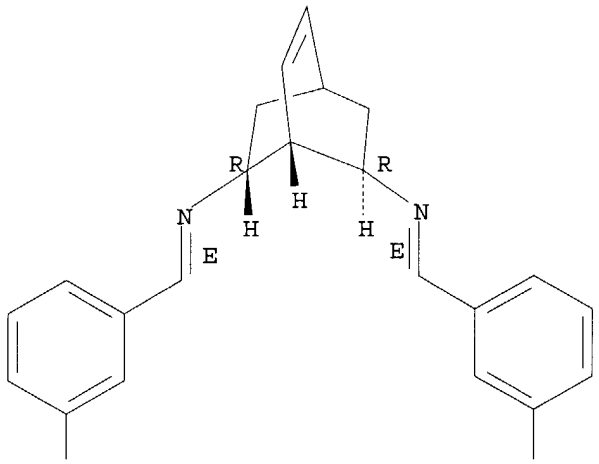
PAGE 2-A



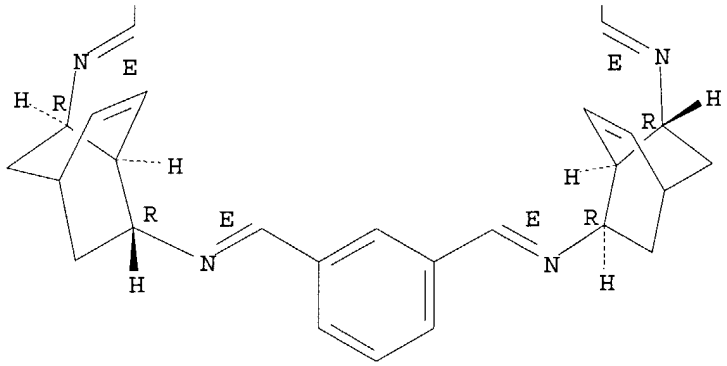
RN 616233-23-9 CAPLUS
CN 3H,14H,28H-3,42:14,17:28,31-Trimethano-7,11:21,25:35,39-trimethenotribenzo[b,n,z][1,5,13,17,25,29]hexaazacyclohexatriacontine, 4,4a,14a,17,18,18a,28a,31,32,32a,42,42a-dodecahydro-, (4aR,5E,12E,14R,18aR,19E,26E,28R,32aR,33E,40E,42R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 2-A



L5 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:427793 CAPLUS
DOCUMENT NUMBER: 129:109446
TITLE: Cyclic oligomer comprising m-phenylene isophthalamide, its metal complex and preparation, a linear homopolymer and copolymer
INVENTOR(S): Kim, Young Hwan; Memeger, Wesley, Jr.
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

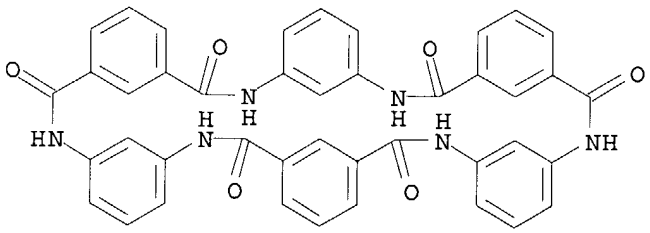
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5770675	A	19980623	US 1996-664898	19960618
US 5969081	A	19991019	US 1998-36130	19980306

PRIORITY APPLN. INFO.: US 1996-664898 19960618
OTHER SOURCE(S): MARPAT 129:109446

AB The title oligomer is prepared by reaction of diacylbenzene with phenylenediamine in solution, preferably in the presence of a metal salt. The aramid products are useful, for example, as fibers for fire resistant clothing. Amino-functional cyclic oligomers may be reacted with polyfunctional acyl halides to produce copolyamides. Thus, isophthaloyl chloride and m-phenylenediamine were dissolved in PhMe and dimethylacetamide (I), resp., and the solution mixed into I containing CaCl2 over 1 h and stirred and precipitated in MeOH/H2O to give a cyclic trimer complex.

IT **172917-20-3DP**, iron complexes **209673-32-5P 209673-33-6P 209673-34-7P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(cyclic oligomer comprising m-phenylene isophthalamide and polymerization)

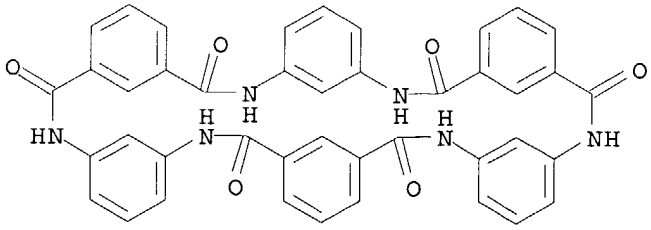
RN 172917-20-3 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-3,9,17,23,31,37-hexone (9CI) (CA INDEX NAME)



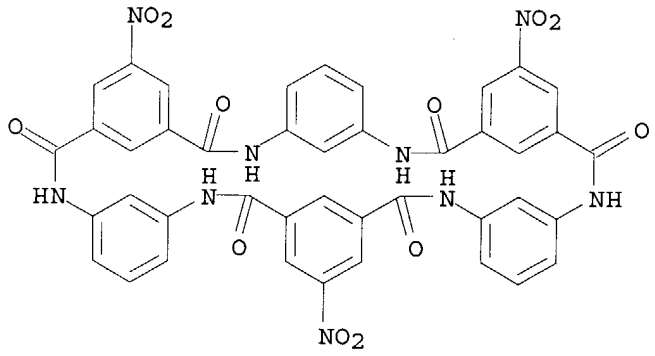
RN 209673-32-5 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-3,9,17,23,31,37-hexone, homopolymer (9CI) (CA INDEX NAME)

CM 1

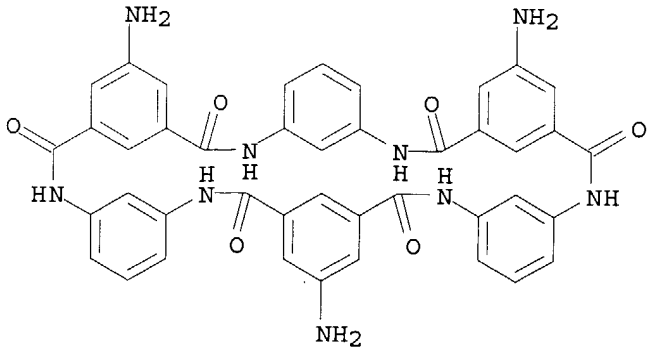
CRN 172917-20-3
CMF C42 H30 N6 O6



RN 209673-33-6 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-3,9,17,23,31,37-hexone, 6,20,34-trinitro- (9CI) (CA INDEX NAME)



RN 209673-34-7 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-3,9,17,23,31,37-hexone, 6,20,34-triamino- (9CI) (CA INDEX NAME)

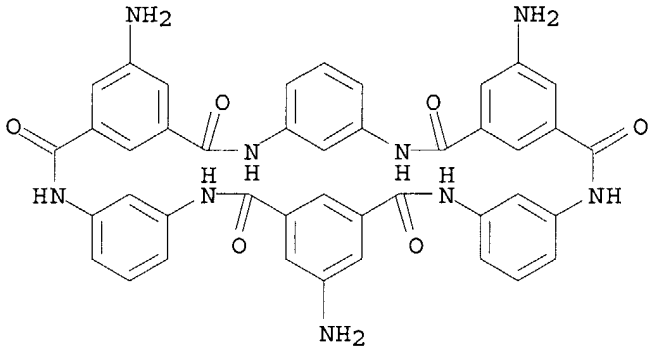


IT **209673-35-8P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(heat-resistant; cyclic oligomer comprising m-phenylene isophthalamide and polymerization)

RN 209673-35-8 CAPLUS
CN 1,4-Benzenedicarbonyl dichloride, polymer with 6,20,34-triamino-2,10,16,24,30,38-hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-3,9,17,23,31,37-hexone (9CI) (CA INDEX NAME)

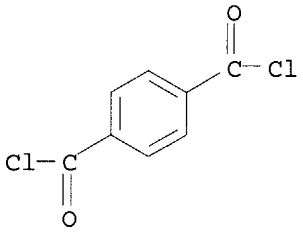
CM 1

CRN 209673-34-7
CMF C42 H33 N9 O6



CM 2

CRN 100-20-9
CMF C8 H4 Cl2 O2

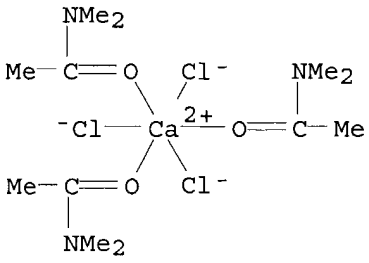


IT **172917-24-7P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and characterization by mass spec and x-ray; cyclic oligomer comprising m-phenylene isophthalamide and polymerization)
RN 172917-24-7 CAPLUS
CN Calcium(2+), tetrakis(N,N-dimethylacetamide-O)bis(2,10,16,24,30,38-hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-3,9,17,23,31,37-hexone-O3)-, (OC-6-11)-, bis[(OC-6-22)-trichlorotris(N,N-dimethylacetamide-O)calciate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 172917-23-6
CMF C12 H27 Ca Cl3 N3 O3

CCI CCS



CM 2

CRN 172917-22-5
CMF C100 H96 Ca N16 O16
CCI CCS

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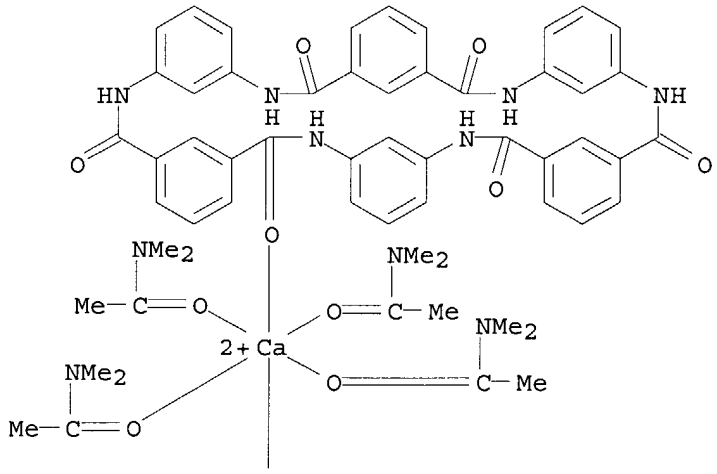

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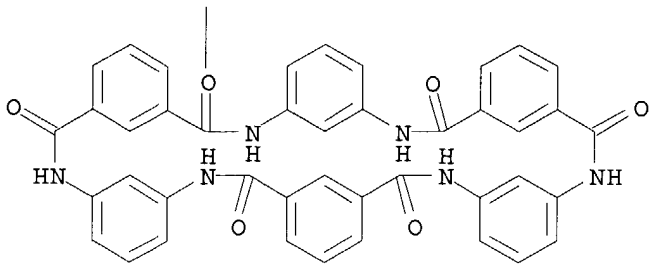
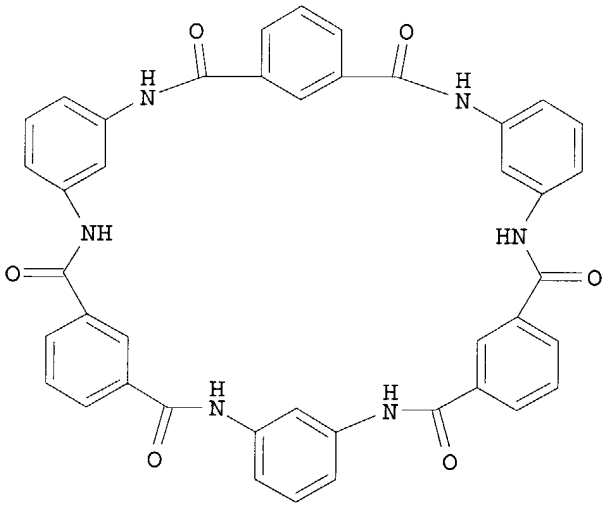


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:61308 CAPLUS
DOCUMENT NUMBER: 124:133805
TITLE: CaCl3- or Ca2Cl4 Complexing Cyclic Aromatic Amide. Template Effect on Cyclization
AUTHOR(S): Kim, Young H.; Calabrese, Joseph; McEwen, Charles
CORPORATE SOURCE: DuPont Central Research and Development, Wilmington, DE, 19880, USA
SOURCE: Journal of the American Chemical Society (1996), 118(6), 1545-6
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

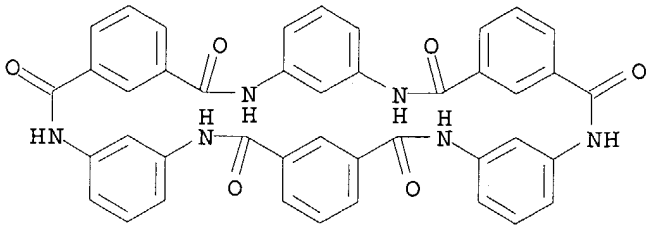


I

AB Cyclic aromatic amides were prepared under high dilution conditions from isophthalic acid chloride and m-phenylenediamine. The most abundant cyclic product is the hexamer (I), which has a chair conformation and forms complexes with CaCl3- or Ca2Cl4 depending on the crystallization conditions, as found by x-ray crystallog. With respect to the CaCl3- complex, all the amide N-H groups are pointing inward and H bonded to Cl-, while the Ca2+ ion is solvated with the carbonyl O atoms of the cyclic amide and DMAc. For the CaCl2 complex, two of the carbonyl groups are pointing inward and coordinate to the Ca ion. This structure is related to a proposed structure for LiCl complexed aromatic polyamide. CaCl2 and other salts that can readily form octahedral complex anion complexes have a template effect on the cyclization. Thus, the yield of cyclic hexamer was increased by .apprx.4-fold when cyclization was carried out in the presence of FeCl3.

IT **172917-20-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with calcium)

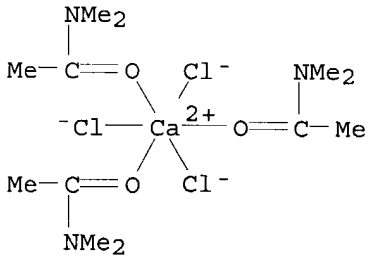
RN 172917-20-3 CAPLUS
CN 2,10,16,24,30,38-Hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-3,9,17,23,31,37-hexone (9CI) (CA INDEX NAME)



IT **172917-24-7P 172917-26-9P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
RN 172917-24-7 CAPLUS
CN Calcium(2+), tetrakis(N,N-dimethylacetamide-O)bis(2,10,16,24,30,38-hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-3,9,17,23,31,37-hexone-O3)-, (OC-6-11)-, bis[(OC-6-22)-trichlorotris(N,N-dimethylacetamide-O)calciate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 172917-23-6
CMF C12 H27 Ca Cl3 N3 O3
CCI CCS



CM 2

CRN 172917-22-5
CMF C100 H96 Ca N16 O16
CCI CCS

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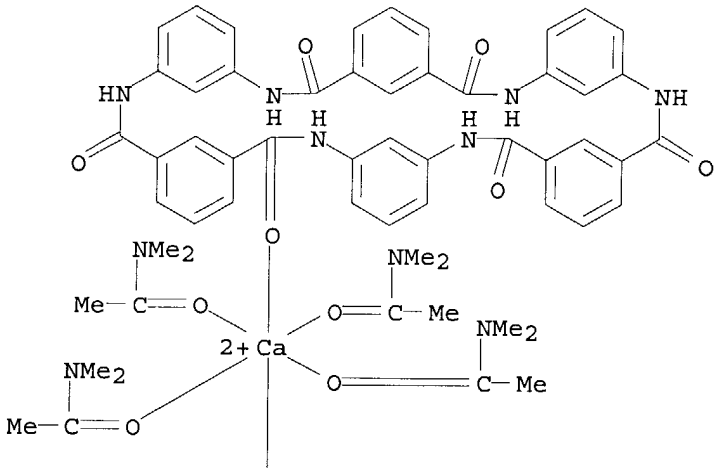

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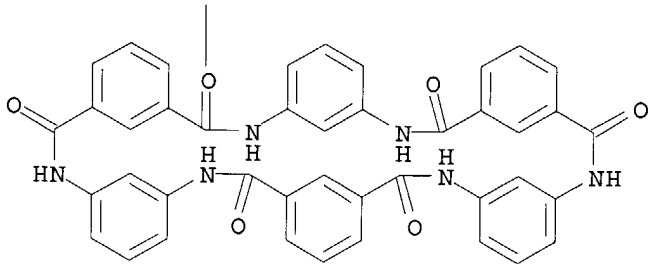

RN 172917-26-9 CAPLUS
CN Calcium, di-μ-chlorodichlorotetrakis(N,N-dimethylformamide-O)bis(2,10,16,24,30,38-hexaazaheptacyclo[37.3.1.14,8.111,15.118,22.125,29.132,36]octatetraconta-1(43),4,6,8(48),11,13,15(47),18,20,22(46),25,27,29(45),32,34,36(44),39,41-octadecaene-3,9,17,23,31,37-hexone-O3,O37)di-, compd. with tetrahydrofuran (1:6) (9CI) (CA INDEX NAME)

CM 1

CRN 172917-25-8
CMF C96 H88 Ca2 Cl4 N16 O16
CCI CCS

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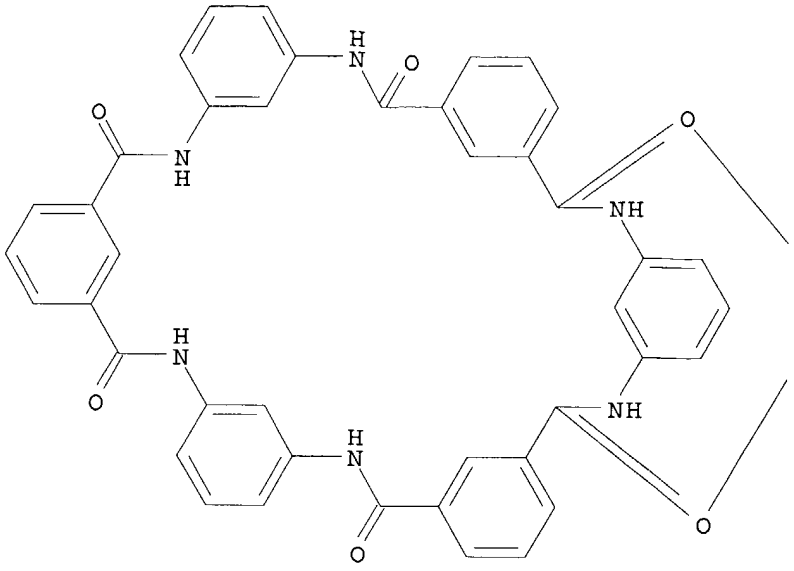

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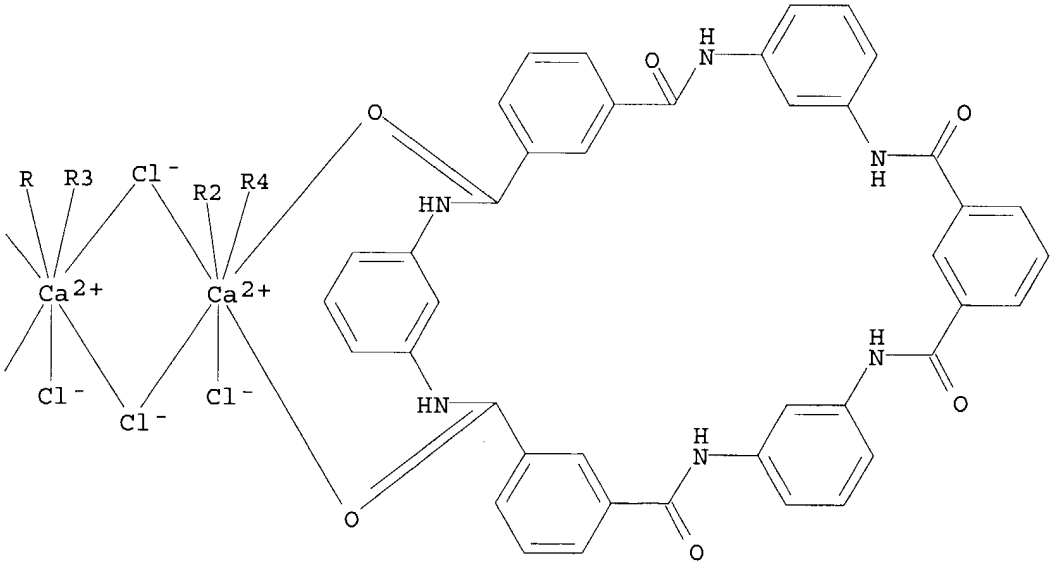

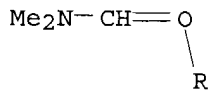

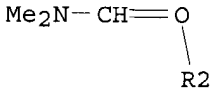

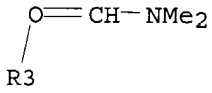

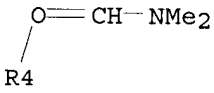

CM 2

CRN 109-99-9
CMF C4 H8 O